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UNIV-MADISON DEPT OF ENGINEERING MECHANICS D S MALKUS
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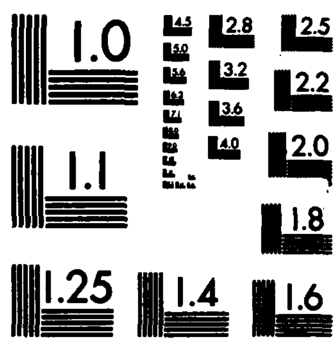

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The project involves the development of efficient and robust finite element scheme for the solution of fluid flow problems in which the stresses are given by an integral constitutive equation. During the second year of the grant progress has been made in the improvement of the computational efficiency of the stress calculator, which is the heart of the method. First, a simple adaptive memory quadrature scheme has been implemented; second the code has been vectorized and tested in vector-processing environments; third, the code has been streamlined by using local array storage instead of regeneration of

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elemental quantities. The improvements lead to a factor of two reduction in running time in the most favorable case tested and to a 40% reduction in the least favorable case, with scalar processing. In vector processing an additional 11% reduction in CPU time is observed.

Progress has been made in the understanding of convergence difficulties at high Weissenberg numbers by analysis of a simple model problem and its discretization. New aspects of the mathematical nature of simple flows of viscoelastic fluids near and beyond the unsteady transition have been observed, in joint work with J. Nohel (Department of Mathematics, UW) and B. Plohr (Department of Computer Science, UW). Work is in progress to translate these new discoveries into practical modifications of the computational scheme for flows in complex geometries.

AFOSR-TR- 87-0848

A FAST ALGORITHM FOR NON-NEWTONIAN FLOW

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Research Objectives

The principal investigator has been developing a fast and computationally efficient implementation of a new method for the computation of steady flows of viscoelastic fluids with single-integral constitutive equations. The P. I. has developed a new kind of finite element method to solve such problems, which has been implemented, tested, and used to solve problems of physical and practical interest. The method is computationally costly, and before it can take its place as a reliable scientific and engineering tool, the P. I. believes its computational cost must be significantly reduced, its robustness and flexibility improved, and some measure of its accuracy in benchmark problems quantified. The aim of the research is to develop an optimized algorithm which will run on the order of a factor of two faster on scalar-architecture machines than does the current algorithm, and will take full advantage of vectorization on machines with that capability.

During the second year of funded research, progress has been made in two areas: improving the efficiency of the central core of the algorithm, the stress calculator, and in a theoretical understanding of the nature of numerical difficulties which arise with some constitutive equations when the stress calculator is used to solve steady boundary-value problems. It is becoming ever more apparent that the two issues can be separated. It is expected that that the major contribution of the current research will be the development of a robust and efficient stress calculator based on linear crossed triangles. Such a stress calculator has merit in its own right and can be employed with a variety of constitutive equations and with a variety of numerical schemes for the solution of the equations of steady motion of the fluid. One such scheme is the one the P. I. has been developing, which uses the crossed-triangle elements themselves to develop a pseudotime Galerkin method. This scheme works well with some constitutive equations: Deborah numbers (non-dimensional flow rates) in excess of 25 can be achieved with a Curtiss-Bird model, Deborah numbers on the order of 5 with a Wagner/Johnson-Segalman fluid, on the order of 3 with an Oldroyd-B

fluid, but only order 1 with a Maxwell fluid, where the "high Weissenberg number problem" seems most severe. It seems appropriate that future work have two relatively independent goals: first to complete the development and documentation of the stress calculator as an independent, portable code of use for solving boundary value problems by the P. I.'s, or alternative methods, or of use for computing stresses in given velocity fields for their own intrinsic interest; second, to continue to investigate the nature of the high Weissenberg problem with the aim of improving the current algorithm or devising improved ones. The first goal is well in sight and can be achieved in the final year of the grant. The second one will probably require a longer-term investigation.

Status of the Research

During the reporting period, research progress has been made in several areas:

1. Vectorization of the fast algorithm: The vectorization of the P. I.'s code for the University of Minnesota Cray-2 has been completed. The result is that the Navier-Stokes code option runs 35% faster, and the non-Newtonian option runs about 11% faster. These figures are in line with what is to be expected, since the non-Newtonian calculation involves mostly element-level calculation with small arrays. A version of the code was also tested on a Cyber 205, and similar cost savings were observed when the code was vectorized for that machine.

2. Code streamlining: In current supercomputing environments core storage capacity is enormous with respect to the needs of the P. I.'s code; this is also true in virtual memory environments. It has proved extremely cost-effective to avoid regeneration of element-level quantities wherever possible, in favor of arrays which are permanent or redefined only at the outset of each iteration. Unlike standard finite element procedures, those for memory fluids must repeatedly use information which is nonlinearly dependent on the current the velocity field at the current time step. For standard finite element procedures, the choice is to generate the information as needed, discarding the result after it is used. Here, it pays to generate element data such as strain rate and save it in a large array at the outset of each inner iteration at each pseudotime step. Since each element can contain the pathlines of many material points required to compute the new stress field, numerous regenerations of the data from nodal values can be avoided. For the P. I. 's code the saving attributable to this trade-off was found to be 20% to compute a solution in abrubt contraction flow for a Johnson-Segalman/Wagner fluid at Deborah number 5.

3. Adaptive memory quadrature. It was discovered that the destabilization of the iteration scheme due to adaptive quadrature reported in the final report for year one of the grant resulted from a coding oversight. This has been corrected, and it has been found that a

factor of two reduction in running time can be obtained with the Maxwell fluid model from the adaptive quadrature alone. As explained in the final report for year one, the saving is less for more complicated constitutive equations but still is significant. For the Johnson-Segalman/Wagner fluid in abrupt contraction flow at Deborah number 5, the saving due to adaptive quadrature was found to be about 20%. Note that the combined savings of items 2. and 3. amount to a reduction of 40% in CPU cost in the Johnson-Segalman/Wagner case and much more in the Maxwell fluid case. Though the improvements of item 2. have yet to be implemented in the supercomputer code, an additional 10% reduction seems to be expectable from vectorization.

4. Model problems for the High Weissenberg Number Problem. The 'HWNP' (High Weissenberg Number Problem) cause difficulty in converging to solutions with significant non-Newtonian effect when many constitutive equations are employed. The P. I. has succeeded in developing two simple, analytically tractable models which seem to show the sources of the HWNP. The resolution seems to be that the combined equations of steady motion and stress are losing their ellipticity with increasing flow rate. This can be treated in 1-D by techniques that are closely related to optimal upwinding techniques for the Navier-Stokes equations. In two space dimensions the problem is more difficult: Added viscosity must be anisotropic; previous attempts to add 'Newtonian' viscosity seem to have failed for this reason. It is also unclear how to define a 'Peclet-like' number for planar flows; anisotropy indicates that there should be at least two of them. This problem is discussed in ref. 5.

5. Added Anisotropic Viscosity. A new method of computing an the added viscosity of item 4. seems to be in the offing. It is based on a correspondence between an incremental effective viscosity and complex viscosity as a function of the in-plane variables taken as a complex variable. The 'Peclet-like' number is computed by contour integration in the complex plane and is itself a complex number whose real and imaginary parts determine in-phase (diagonal) and out-of-phase (off-diagonal) contributions to the added viscosity. This procedure has been applied to a linear non-constant coefficient problem (eq. (28) of ref. 5) and has been found to improve the convergence rate of the iterative method for that model problem. However, to date, similar success has not been acheived in the nonlinear, memory-dependent case, and it is clear that further investigation is reqired.

The P. I. has been involved in a joint investigation of the mathematical nature of some simple model problems in viscoelastic flow with J. Nohel (Dept. Mathematics, UW) and B. Plohr (Dept. Computer Science, UW). These investigations lead beyond the scope of the P. I.'s research under the current AFOSR grant, and we are attempting to find independent sources of funding for them. We have, however, discovered some interesting mathematical aspects of the model problems which we hope will be relevant to the current grant research in the coming year. We hope our investigations will lead us to an understanding of the

added Newtonian viscosity approach, or lead us to some substitute for it. We also find that the loss of ellipticity in the steady equations corresponds to a transition to unsteady flow which is distinct from the onset of Hadamard instability. It seems that regimes of unsteady flow or perhaps regimes of steady flows with singularities may exist beyond the transition. It could well be that the HWNP is telling us that the flows in question 'want' to be unsteady and that the current method for steady flows may be doing as well as can be hoped for, under the circumstances. Added viscosity may allow us to compute somewhat closer to the unsteady transition, but new approaches are demanded beyond transition. The P. I hopes that the stress calculation procedure developed under the current grant will at least be useful in regimes where steady flows are known to exist and that it may even prove useful for new methods which can proceed beyond transition.

Publications

Journal Articles Appearing During Reporting Period

1. with M. F. Webster, "On the accuracy of finite element and finite difference predictions of non-Newtonian slot pressures for a Maxwell fluid," in press, **J. Non-Newtonian Fluid Mechanics.**

Journal Articles Submitted During Reporting Period

2. With M. E. Plesha and M.-R. Liu, "Reversed stability conditions in transient finite element analysis," MRC Technical Summary Report No. 2971, Mathematics Research Center, University of Wisconsin-Madison (1987), submitted to **Comp. Meths. Appl. Mechs. Eng.**

3. With X. Qiu, "Divisor structure of finite element eigenproblems arising form negative and zero masses," MRC Technical Summary Report No. 2969, Mathematics Research Center, University of Wisconsin-Madison (1987), submitted to **Comp. Meths. Appl. Mechs. Eng.**

Unpublished Reports During Reporting Period

4. With Minwu Yao, "On hole-pressures in plane Poiseuille flow over transverse slots," MRC Technical Summary Report No. 2943, Mathematics Research Center, University of Wisconsin-Madison (1986).

5. "Computational methods for viscoelastic flow," uncatalogued Mathematics Research Center Report, University of Wisconsin-Madison (1987).

Articles/Reports in Progress

6. with M. F. Webster, "Numerical Evaluation of an empirical measurement relation for non-Newtonian slot pressures."

Interactions

Spoken Papers Presented at Meetings, Conferences, Seminars, etc.

1. "On the accuracy of finite element and finite difference predictions of non-Newtonian slot pressures for a Maxwell fluid," Workshop on Computational Fluid Dynamics and Reacting Gas Flows, Institute for Mathematics and Its Applications, Minneapolis, September, 1986 (resulting in ref. 1, above).

2. Two-week lecture series on "The finite element method in structural and continuum mechanics," Nanjing Aeronautical Institute, Nanjing, P. R. C. (led to ref. 3, above).

Consultative and Advisory Functions

1. The P. I. has maintained a close advisory relationship with the non-Newtonian fluids group at Illinois Institute of Technology, headed by B. Bernstein. The pilot method was developed jointly with Bernstein during the six years the P. I. was on the mathematics faculty at I. I. T. The P. I. has been working closely with E. T. Olsen on the development of the stress calculator. The P. I. continues to make regular visits to I. I. T. for the purpose

of co-ordinating the research effort. He served on the Ph. D. Thesis committee of Dr. Alan Altman, who recently received his Ph. D. under E. T. Olsen. His research involved the development of a temperature-dependent material clock for the stress calculator.

2. The P. I. continues to collaborate closely with A. S. Lodge (Dept. Engineering Mechanics, U. W. - Madison), who has developed a laboratory measurement device for normal-stress differences and viscosities based on hole-pressures. The collaboration provides an opportunity for the P. I. to relate his numerical studies to experimental results, and has provided Prof. Lodge with independent verification of the empirical measurement relation upon which his instrument relies.

3. The P. I. continues as a member of the Executive Committee of the Rheology Research Center (U. W. - Madison). This provides a valuable opportunity to interact with a broad spectrum of reasearchers in non-Newtonian mechanics from Mathematics Chemistry, Engineering Mechanics, and Chemical Engineering.

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